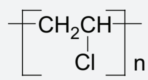
# PVC poly(vinyl chloride)

| PARAMETER | UNIT | VALUE | REFERENCES |
|---|---|---|---|
| **GENERAL** | | | |
| **Common name** | - | poly(vinyl chloride) | |
| **IUPAC name** | - | poly(chloroethanediyl) | |
| **CAS name** | - | ethene, chloro-, homopolymer | |
| **Acronym** | - | PVC | |
| **CAS number** | - | 9002-86-2 | |
| **EC number** | - | 208-750-2 | |
| **RETECS number** | - | KV0350000 | |
| **Formula** | |  | |
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| **HISTORY** | | | |
| **Person to discover** | - | Henri Victor Regnault (accidental polymerization), Fritz Klatte (technological developments), Waldo Semon (commercial applications | |
| **Date** | - | 1835, beginning of 20th century, 1926 | |
| **Details** | - | Henri Victor Regnault observed that vinyl monomer forms white solid material when exposed to sunlight; Klatte worked on processability; Semon continued Klatte efforts and succeeded in plasticization; extensive commercial applications had to wait on development of thermal stabilizers, which permitted industrial processing during Second World War in US | |
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| **SYNTHESIS** | | | |
| **Monomer(s) structure** | - | $H_2C{=}CHCl$ | |
| **Monomer(s) CAS number(s)** | - | 75-01-4 | |
| **Monomer(s) molecular weight(s)** | dalton, g/mol, amu | 62.498 | |
| **Monomer ratio** | - | 100% | |
| **Formulation example** | - | suspension: water, suspending agent, initiator; emulsion: water, emulsifier, water-soluble initiator; microsuspension: water, emulsifier, oil-soluble initiator; bulk: initiator | |
| **Common initiators** | | tert-octyl peroxyneodecanoate, dicyclohexyl peroxydicarbonate, tert-butyl peroxyneodecanoate, benzoyl peroxide, 2,2'-azobisbutylnitrile, tert-amyl peroxypivalate, dilauroyl peroxide | |
| **Method of synthesis** | - | suspension, microsuspension, emulsion, bulk | |
| **Temperature of polymerization** | $^oC$ | 55-73 | |
| **Yield** | % | 80-90 | |
| **Heat of polymerization** | kJ $mol^{-1}$ | -96 to -109 | |
| **Typical concentration of residual monomer** | ppm | <1 | |
| **Mass average molecular weight, $M_w$** | dalton, g/mol, amu | 37,000-214,000 | |
| **Polydispersity, $M_w/M_n$** | - | 1.90-2.59 (suspension); 2.14-2.65 (emulsion); 2.00-2.06 (mass) | |
| **Polymerization degree (number of monomer units)** | - | 600-3,400 | |
| **K number** | | 50-95 (suspension); 60-80 (emulsion); 58-69 (mass) | |

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| **Mean particle size** | μm | 100-150 (suspension); 40-50 (general purpose emulsion); 2-25 (paste forming) | |
| **Molar volume at 298K** | $cm^3$ $mol^{-1}$ | calc.=41.0 (crystalline); 45.1-58.4 (amorphous) | |
| **Van der Waals volume** | $cm^3$ $mol^{-1}$ | calc.= 29.2 (crystalline); 29.2-38.0 (amorphous) | |
| **Molecular cross-sectional area, calculated** | $cm^2$ x $10^{-16}$ | 18.5 | |
| **Radius of gyration** | nm | 5-10; 16.4-28.2 | Wan, C; Qiao, X; Zhang, Y; Zhang, Y, Polym. Test., 22, 453-61, 2003; Mutin, P H; Guenet, J M, Polymer, 27, 7, 1098-1102, 1986. |
| **Degree of branching** | number/ 1000 VC | 3.3-4.8 (chloromethyl), 0.8 (short branches from backbiting, 0.1-0.2 (long branches), 0.9 (tertiary chlorines) | |
| **Unsaturations** | number/ 1000 VC | 0.1-0.3 (internal allylic chlorine), 0.1-0.6 (internal), 0.75-0.8 (end-group), 0.95-1.7 (total) | |
| **Typical chain imperfections** | number/ 1000 VC | 6-8 (head-to-head), 0.1-0.4 (initiator rests) | |
| | | | |
| **STRUCTURE** | | | |
| **Crystallinity** | % | 4-10 (commercial) | |
| **Crystalline structure** | - | lamellar, fringed micelles | |
| **Cell type (lattice)** | - | orthorhombic | |
| **Cell dimensions** | nm | a:b:c=1.01-1.08:0.53-0.54:0.510-0.512 | Natta, G; Corradini, P, J. Polym. Sci., 20, 251, 1956. |
| **Unit cell angles** | degree | $\alpha$:$\beta$:$\gamma$=90:90:90 | |
| **Number of chains per unit cell** | - | 2 | Natta, G; Corradini, P, J. Polym. Sci., 20, 251, 1956. |
| **Crystallite size** | nm | 0.7-15 | |
| **Spacing between crystallites** | nm | 0.36; 0.5 | |
| **Tacticity** | % | 55-68 (syndiotactic dyads); typical: 27.6-44.0 (syndiotactic), 4.8-21.8 (isotactic), 30.5-52.0 ((heterotactic) | |
| **Chain conformation** | - | planar zigzag | |
| **Entanglement molecular weight** | dalton, g/ mol, amu | 6,250 | |
| **Lamellae thickness** | nm | 2.5-6 | Ballard, D G H; Burgess, A N; Deconinck, J W; Roberts, E A, Polymer, 28, 1, 3-9, 1987. |
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| **COMMERCIAL POLYMERS** | | | |
| **Some manufacturers** | - | PolyOne | |
| | | | |
| **PHYSICAL PROPERTIES** | | | |
| **Density at 20°C** | g $cm^{-3}$ | 1.37-1.43; 1.53 (crystalline); 1.373 (amorphous) | |
| **Bulk density at 20°C** | g $cm^{-3}$ | 0.39-0.59 | |
| **Color** | - | white | |
| **Refractive index, 20°C** | - | 1.532-1.548 | |
| **Odor** | - | odorless | |
| **Melting temperature, DSC** | °C | 103-230; 400 (syndiotactic, estimate) | |
| **Decomposition onset temperature** | °C | 200 | Patel, P; Hull, T R; McCabe, R W; Flath, D; Grasmeder, J; Percy, M, Polym. Deg. Stab., 95, 709-18, 2010. |

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|---|---|---|---|
| **Fusion temperature** | $^oC$ | 185-195 | |
| **Thermal expansion coefficient, 23-80$^oC$** | $^oC^{-1}$ | 3.5-7.1E-5 | |
| **Thermal conductivity, melt** | W $m^{-1}$ $K^{-1}$ | 0.13-0.17 | |
| **Glass transition temperature** | $^oC$ | calc.=81-82; exp.=82-87 (rigid); 66 (5 phr plasticizer); 13-52 (30 phr plasticizer); -52 to -82 (100 phr plasticizer) | |
| **Specific heat capacity** | J $K^{-1}$ $kg^{-1}$ | 900-970 | |
| **Heat deflection temperature at 1.8 MPa** | $^oC$ | 73-74 | |
| **Vicat temperature VST/A/50** | $^oC$ | 82-95 | |
| **Vicat temperature VST/B/50** | $^oC$ | 65-100 | |
| **Hansen solubility parameters, $\delta_D$, $\delta_P$, $\delta_H$** | $MPa^{0.5}$ | 18.82, 10.03, 3.07; 16.8, 8.9, 6.1; 18.4, 6.6, 8.0 | |
| **Interaction radius** | | 8.5; 3.5; 3.0 | |
| **Molar volume** | kmol $m^{-3}$ | 45.2 | |
| **Hildebrand solubility parameter** | $MPa^{0.5}$ | calc.=19.28-20.23; exp.=19.19-20.1 | |
| **Surface tension** | mN $m^{-1}$ | 32-46 | Wu, S, J. Adhesion, 5, 39, 1973. |
| **Dielectric constant at 1 kHz/1 MHz** | - | 3.39-3.5 | |
| **Dielectric loss factor at 1 kHz** | - | 0.81 | |
| **Relative permittivity at 100 Hz** | - | 0.009-0.017 | |
| **Volume resistivity** | ohm-m | 1E12 to 1E13 | |
| **Surface resistivity** | ohm | 1E11 to 1E12 | |
| **Arc resistance** | s | 60-80 | |
| **Coefficient of friction** | - | 0.35-0.8 (static), 0.72-0.93 (dynamic) on steel | DeCoste, J B, Antec, 232, 1969. |
| **Permeability to nitrogen, 25$^oC$** | $m^3$ $s^{-1}$ $m^2$ $Pa^{-1}$ $10^{-9}$ | 0.0089 | |
| **Permeability to oxygen, 25$^oC$** | $m^3$ $s^{-1}$ $m^2$ $Pa^{-1}$ $10^{-9}$ | 0.034 | |
| **Permeability to water vapor, 25$^oC$** | $m^3$ $s^{-1}$ $m^2$ $Pa^{-1}$ $10^{-9}$ | 0.12 | |
| **Diffusion coefficient of nitrogen** | $cm^2$ $s^{-1}$ $x10^6$ | 0.0038 | |
| **Diffusion coefficient of oxygen** | $cm^2$ $s^{-1}$ $x10^6$ | 0.012 | |
| **Contact angle of water, 20$^oC$** | degree | 83.2-91.9 | |
| **Surface free energy** | mJ $m^{-2}$ | 40.1 | |
| **Speed of sound** | m $s^{-1}$ | 39.7 | |
| **Acoustic impedance** | | 3.27 | |
| **Attenuation** | dB $cm^{-1}$, 5 MHz | 11.2 | |
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| **MECHANICAL & RHEOLOGICAL PROPERTIES** | | | |
| **Tensile strength** | MPa | 7.1-68.9 | |
| **Tensile modulus** | MPa | 2,430-4,000 | |
| **Tensile stress at yield** | MPa | 39.2-88.3 | |
| **Elongation** | % | 3.3-430 | |

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|---|---|---|---|
| **Flexural strength** | MPa | 67-107 | |
| **Flexural modulus** | MPa | 2,580-3,310 | |
| **Tear strength** | MPa | 2.1-7.9 | |
| **Izod impact strength, notched, 23°C** | J $m^{-1}$ | 33-1302 | |
| **Tenacity (fiber) (standard atmosphere)** | cN $tex^{-1}$ (daN $mm^{-2}$) | 10-30 | Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999. |
| **Tenacity (wet fiber, as % of dry strength)** | % | 100 | Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999. |
| **Fineness of fiber (titer)** | dtex | 1.5-60 | Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999. |
| **Length (elemental fiber)** | mm | 38-200 | Fourne, F, Synthetic Fibers. Machines and Equipment Manufacture, Properties. Carl Hanser Verlag, 1999. |
| **Poisson's ratio** | - | 0.380-0.385 | |
| **Shore A hardness** | - | 30-96 | |
| **Shore D hardness** | - | 22-25 | |
| **Rockwell hardness** | - | M66-69 | |
| **Shrinkage** | % | 0.5-2.5 | |
| **Brittleness temperature (ASTM D746)** | °C | -29 to -41 | |
| **Water absorption, equilibrium in water at 23°C** | % | 0.04-0.4 | |
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| **CHEMICAL RESISTANCE** | | | |
| **Acid dilute/concentrated** | - | very good | |
| **Alcohols** | - | good | |
| **Alkalis** | - | very good | |
| **Aliphatic hydrocarbons** | - | good | |
| **Aromatic hydrocarbons** | - | fair-poor | |
| **Esters** | - | poor | |
| **Greases & oils** | - | good | |
| **Halogenated hydrocarbons** | - | poor | |
| **Ketones** | - | poor | |
| **Q solvent, Θ-temp.=155.4, 22, 36.5, 84°C** | - | benzyl alcohol, cyclohexanone, dimethylformamide, o-xylene | |
| **Good solvent** | - | chlorobenzene, cyclohexanone, DMF, DMSO, MEK, nitrobenzene, THF | |
| **Non-solvent** | - | acetone, non-oxidizing acids, alkalies, aniline, carbon disulfide, hydrocarbons, nitroparaffins | |
| **Effect of EtOH sterilization (tensile strength retention)** | % | 113-115 | Navarrete, L; Hermanson, N, Antec, 2807-18, 1996. |
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| **FLAMMABILITY** | | | |
| **Ignition temperature** | °C | 391 | |

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|---|---|---|---|
| **Autoignition temperature** | $^o$C | 435-454 | |
| **Limiting oxygen index** | % $O_2$ | 37-49 | |
| **Heat release** | kW $m^{-2}$ | 176 | Yu, B; Liu, M; Lu, L; Dong, X; Gao, W; Tang, K, Fire Mater., 34, 251-61, 2010. |
| **NBS smoke chamber** | Ds | 349-500 | Padey, D; Walling, J; Wood A, Polymers in Defence and Aerospace 2007, Rapra, 2007, paper 15. |
| **Char at 500$^o$C** | % | 10.9-18.0 | Lyon, R E; Walters, R N, J. Anal. Appl. Pyrolysis, 71, 27-46, 2004. |
| **Heat of combustion** | J $g^{-1}$ | 17,950 | |
| **Volatile products of combustion** | - | CO, $CO_2$, $H_2O$, HCl; traces of benzene and phosgene | |
| **CO yield** | % | 8 (with flame retardant) | |
| | | | |
| **WEATHER STABILITY** | | | |
| **Spectral sensitivity** | nm | 310-370 | |
| **Activation wavelengths** | nm | 310-325, 327, 364 | |
| **Excitation wavelengths** | nm | 284, 290 | |
| **Emission wavelengths** | nm | 350, 440 | |
| **Activation energy of photoxidation** | kJ $mol^{-1}$ | 32.1 (nitrogen); 19.6 (air) | |
| **Depth of UV penetration** | $\mu$m | 90; 150-200 | |
| **Important initiators and accelerators** | - | carbonyl groups, unsaturations, solvents forming hydroperoxides, sensitizing impurities (e.g., benzophenones), metaloorganics (copper-containing compounds, cadmium acetate, ferrocene, iron salts), metal chlorides produced from thermal stabilizers, products of degradation of some antioxidants, some pigments and fillers (containing cobalt, zinc, manganese, and lead), metal oxides (of titanium, zinc, and aluminum), hydrogen chloride (autocatalytic product of PVC degradation) | |
| **Products of degradation** | - | free radicals, unsaturations, carbonyl groups, hydroperoxides, chain scissions, crosslinks | |
| **Stabilizers** | | UVA: 2-hydroxy-4-octyloxybenzophenone; 2-hydroxy-4-methoxybenzophenone; 2,2'-dihydroxy-4-methoxybenzophenone; 2-(2H-benzotriazol-2-yl)-p-cresol; 2-benzotriazol-2-yl-4,6-di-tert-butylphenol; 2-(2H-benzotriazole-2-yl)-4,6-di-tert-pentylphenol; 2-(2H-benzotriazole-2-yl)-4-(1,1,3,3-tetraethylbutyl) pheno; 2-(2H-benzotriazol-2-yl)-6-dodecyl-4-methylphenol, branched & linear; reaction product of methyl 3(3-(2H-benzotriazole-2-yl)-5-t-butyl-4-hydroxyphenyl propionate/PEG 300; ethyl-2-cyano-3,3-diphenylacrylate; (2-ethylhexyl)-2-cyano-3,3-diphenylacrylate; N-(2-ethoxyphenyl)-N'-(2-ethylphenyl) oxamide; propanedioic acid, [(4-methoxyphenyl)-methylene]-dimethyl ester; Screener: carbon black, titanium dioxide, zinc oxide; Acid scavenger: hydrotalcite; | |

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|---|---|---|---|
| **Stabilizers (continuation)** | - | HAS: 1,3,5-triazine-2,4,6-triamine, N,N'''[1,2-ethane-diyl-bis[[[4,6-bis[butyl(1,2,6,6-pentamethyl-4-piperidinyl) amino]-1,3,5-triazine-2-yl]imino]-3,1-propanediyl]bis[N',N''-dibutyl-N',N''-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-; bis(1,2,2,6,6-pentamethyl-4-piperidyl) sebacate and methyl 1,2,2,6,6-pentamethyl-4-piperidyl sebacate; bis(1,2,2,6,6-pentamethyl-4-piperidyl)sebacate + methyl-1,2,2,6,6-pentamethyl-4-piperidyl sebacate; bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate; poly[[(6-[1,1,3,3-tetramethylbutyl)amino]-1,3,5-triazine-2,4-diyl][2,2,6,6-tetramethyl-4-piperidinyl)imino]-1,6-hexanediyl[2,2,6,6-tetramethyl-4-piperidinyl)imino]]; C20-24-.alpha.-, polymers with maleic anhydride, reaction products with 2,2,6,6-tetramethyl-4-piperidinamine; 1,6-hexanediamine, N,N'-bis(2,2,6,6-tetramethyl-4-piperidinyl)-, polymers with morpholine-2,4,6-trichloro-1,3,5-triazine reaction products, methylated; Phenolic antioxidants: ethylene-bis(oxyethylene)-bis(3-(5-tert-butyl-4-hydroxy-m-tolyl)-propionate); pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate); 3,3',3',5,5',5'-hexa-tert-butyl-a,a',a'-(mesitylene-2,4,6-triyl) tri-p-cresol; 1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione; isotridecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate; 2,2'-ethylidenebis (4,6-di-tert-butylphenol); 3,5-bis(1,1-dimethyethyl)-4-hydroxy-benzenepropanoic acid, C13-15 alkyl esters; 1,1,3-tris(2'methyl-4'-hydroxy-5'tert-butylphenyl)butane | |
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| **BIODEGRADATION** | | | |
| **Colonized products** | | mattresses, plasticizers | |
| **Typical biodegradants** | - | phthalate esters are degraded by a wide range of bacteria and actinomycetes under both aerobic and anaerobic conditions | |
| **Stabilizers** | - | copper nanoparticle, 4,5-dichloro-2-n-octylisothiazolin-3-one, 2-n-octyl-isothiazolin-3-one, 10,10'-oxybisphenoxarsine, surface azidation,4 tebuconazole, 2,3,5,6-tetrachloro-4-(methylsulphonyl)pyridine, zeolite encapsulated 2-n-octyl-4-isothiazolin-3-one, zinc pyrithione | |
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| **TOXICITY** | | | |
| **NFPA: Health, Flammability, Reactivity rating** | - | 1/1/0 | |
| **Carcinogenic effect** | - | not listed by ACGIH, NIOSH, NTP | |
| **TLV, ACGIH** | mg $m^{-3}$ | 1 (respirable) | |
| **OSHA** | mg $m^{-3}$ | 5 (respirable); 15 (total) | |
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| **ENVIRONMENTAL IMPACT** | | | |
| **Aquatic toxicity, Daphnia magna, $LC_{50}$, 48 h** | mg $l^{-1}$ | 800-8,000; 8,000-235,0000 | Lithner, D; Damberg, J; Dave, G; Larsson, A, Chemosphere, 74, 1195-1200, 2009; Lithner, Ph D Thesis, Univrsity of Gothenburg, 2011. |
| **Cradle to grave non-renewable energy use** | MJ/kg | 53-55 | |
| **Cradle to pellet greenhouse gasses** | kg $CO_2$ $kg^{-1}$ resin | 2.0-2.1 | |
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| **PROCESSING** | | | |
| **Typical processing methods** | - | blow molding, calendering, extrusion, injection molding, plastisol coating, rotational molding, thermoforming | |

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| **Additives used in final products** | - | Fillers: aluminum fiber, aluminum hydroxide, antimony trioxide, calcium carbonate, carbon black, carbon fiber, clay, magnesium hydroxide, montmorillonite, sand, silica, talc, titanium dioxide, wood fiber; Plasticizers: adipates, azelates, benzoates, citrates, epoxidized soybean oil, ethylene interpolymers, phosphates, phthalates, polyester-type polymeric plasticizers, sebacates; Antistatics: chlorinated polyethylene, carbon black, copper powder, ethoxylated fatty dimethyl ethylammoniumethosulfate, glycerol monostearate, graphite, polyethylene glycol monolaurate, propanesultone; Antiblocking: aluminosilicate, natural silica, synthetic silica; Release: ester wax, ethylene N,N'-bisstearamide, glyceryl monostearate; Slip: ethylene N,N'-bisoleamide, stearamide, zinc or calcium stearate or their mixture | |
| **Applications** | - | bottles, cables, coated fabrics, domestic appliances, drain pipes, film and sheet, fittings, flooring, foam backings of carpets, footwear, furniture trim, gloves, gutters, metal protection in automotive, office equipment, packaging, pipes, profiles, protective clothing, toys, tubing, siding, wallpaper, windows, and many more; ranking: high to low: pipe & fitting, window, rigid profile, wire and cable, flexible film, bottles, flooring, coating, flexible tube, roofing, medical, rigid sheet | |
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| **BLENDS** | | | |
| **Suitable polymers** | - | ENR, epoxy, EVA, NBR, NR, PANI, PMMA, PS, PUR, PVA, PVB, PVDF, SAN, SBR | |
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| **ANALYSIS** | | | |
| **FTIR (wavenumber-assignment)** | $cm^{-1}$/- | 1714, 1715, 1718, 1720, 1730 (carbonyl); 1785 (acid chloride); 1510 (carboxylate stabilizer); 3476-3420 (hydroperoxide); 3460 (hydroxyl); 1650 (isolated double bond); 1580 (conjugated double bond) | |
| **Raman (wavenumber-assignment)** | $cm^{-1}$/- | syndiotactic triads – 608, 630, 636; isotactic triads – 697 | Dubault, A; Bokobza, L; Gandin, E; Halary, J L; Polym. Int., 52, 7, 1108-18, 2003. |
| **NMR (chemical shifts)** | ppm | C NMR: $CH_2$ – 46; CHCl – 58 | Colombani, J; Labed, V; Joussot-Dubien, C; Perichaud, A; Raffi, J; Kister, J; Rossi, C, Nuclear Instruments Methods Phys. Rese., B265, 238-44, 2007. |
| **x-ray diffraction peaks** | degree | 16-18, 25 (crystalline area) | |